18. Explain the Hartree-Fock self-consistent field (SCF) method. How does it improve upon the simple approximation of independent electron motion?

19. Construct the character of Irreducible representation and explain the electronic spectra of HCHO.

20. Explain the use of Linear Variation Function and LCAO methods.

Shanmuga Industries Arts Science College T.V.Malai

APRIL/MAY 2025

23PCH42 — PHYSICAL CHEMISTRY — II

Time : Three hours Maximum : 75 marks

SECTION A — (10 × 2 = 20 marks)

Answer ALL questions.

1. Define Wave-Particle Duality.
2. Explain Wave Function.
3. What is anharmonicity.
4. What is degeneracy?
5. Write a short note a Hamiltonian-Wave Equation.
6. Explain Radial and Angular Functions.
7. What are Groups and sub groups.
8. Write an example for Cnh and Dnh group.

9. How does the Heitler-London approach describe the bonding in the hydrogen molecule (H_2)?

10. What is the concept of a Linear Variation Function (LVF) and how is it used in quantum chemistry?

SECTION B — ($5 \times 5 = 25$ marks)

Answer ALL questions.

11. (a) State the postulates of quantum mechanics.

Or

(b) Explain photoelectric effect.

12. (a) Describe the degeneracy of energy levels in a 2D Box.

Or

(b) Describe how the bond length of a diatomic molecule can be determined using rotational Spectroscopy.

13. (a) Discuss the Hartree-Fock self-consistent field method for electronic structure calculations.

Or

(b) Explain the concept of perturbation theory. Apply it to a simple system to illustrate its use.

14. (a) Construct a character table for C_{3v} point group.

Or

(b) Explain the consequences of Great orthogonality theorem.

15. (a) Apply the Huckel method to determine the energy levels and draw the molecular orbital diagrams for benzene.

Or

(b) Explain the results of the Huckel method applied to the cyclobutadiene and calculate its delocalization energy.

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SECTION C — ($3 \times 10 = 30$ marks)

Answer any THREE questions.

16. Explain the time-dependent and time-independent forms of the Schrödinger equation.

17. Write the Schrödinger wave equation for a 1D harmonic oscillator. Discuss solutions, energy levels, and wave functions.